Runge Kutta, Von Neumann, ODEs

PHYS 250 (Autumn 2018) – Lecture 10

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November 6, 2018

Outline

1. *Connection between minimization and solving differential equations*
   - Reminders from Lecture 8
   - Categories of problem
   - Specific example

2. *Finding roots*
   - Bisection method
   - Bisection method

Reminders from last time

There are many examples of optimization in physics

Examples of minimization

- **Fitting a model to data:** minimize differences between a model and data
- **Second law of thermodynamics:** minimize changes in entropy for a system in thermodynamic equilibrium
- **Conservation of momentum:** establish mechanical equilibrium by minimizing changes in momentum, $\frac{d\vec{p}}{dt} = 0$
- **Principle of least action:** obtain the equations of motion of a system by minimizing (or maximizing!) the variations of the action, S
- **Path integral formulation of quantum mechanics:** sort quantum mechanically possible trajectories by minimizing quantum action
- **Ising model:** minimization the energy of the spin configurations

Optimization and root finding

Ultimately, I want to bring us to the point of discussing **optimization in the context of modeling** (c.f. Lecture 1!).

What that means, is that we want to have the computational tools to be able to **model data and approximate complex functions computationally**, since it is often **impossible to do so analytically**.

To achieve that, let's expand our tool kit beyond the analytically solvable example from last time (the 2D linear regression for χ^2 minimization).

Categorizing the problems

As we discussed in Lecture 8, an **optimization problem** quickly turns into an attempt to solve a first-order ordinary (ODE) or partial differential equation (PDE) in order to identify the value of the parameter α for which the function F is stationary:

$$F'(\alpha) = 0 \tag{1}$$

The approaches used to do this are closely related to the methods used for finding zeroes or **"roots"** of functions (since the derivative of a function is, of course, also a function!). But we need to differentiate the problems:

Initial vs. boundary value problems

Imagine you have the ODE

$$F'' = -F \tag{2}$$

- **Initial value problem:** $F(0) = 1, F'(0) = 0$
- **Boundary value problem:** $F(0) = 1, F(\pi) = 0$

The latter is often much harder!

Explicit root finding: square well potential

The Schrodinger equation

$$\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x) \tag{3}$$

tells us that for a finite square-well potential

$$V(x) = \begin{cases} -V_0 & 0 < x < L \\ 0 & \text{else} \end{cases} \tag{4}$$

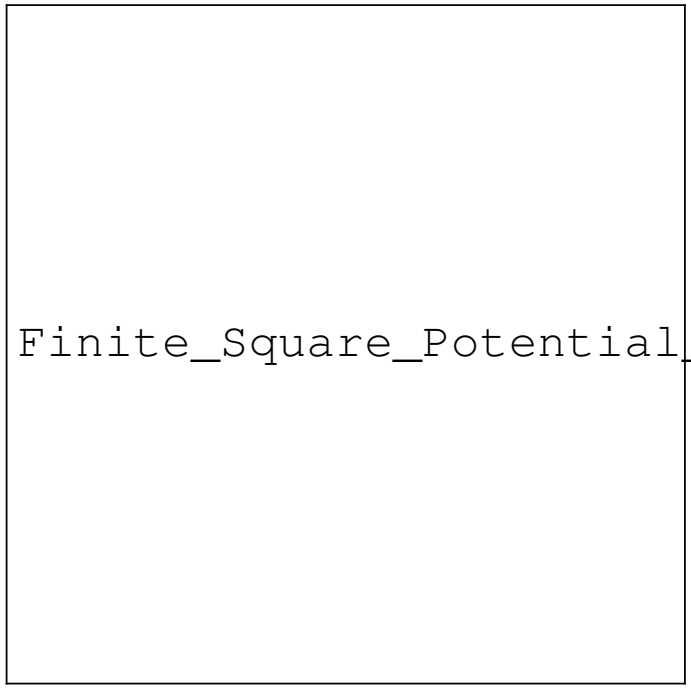
and a bound state ($E = -f < 0, f$ positive definite) in the region $x < 0$, we must solve:

$$-\frac{\hbar^2}{2m}\psi''(x < 0) = -f\psi(x < 0) \tag{5}$$

The solution for $x < 0$ is

$$\psi(x < 0) = Ae^{\sqrt{z_0^2 - z^2}\,x}, \text{ where } z_0^2 - z^2 = \frac{2mf}{\hbar^2} \tag{6}$$

and $z_0^2 \equiv 2mV_0/\hbar^2$.



In order to solve for the bound-state energies, we need to solve the following

$$\tan(za) = \frac{2\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}{2 - \left(\frac{z_0}{z}\right)^2} \tag{7}$$

This is transcendental, requires numerical approaches to finding the **"root"** of

$$2\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

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Bisection method

The bisection method is straightforward and reliable.

Start with an interval defined by its endpoints, x_ℓ and x_r on the left and right of a starting point, such that

$$F(x_\ell)F(x_r) < 0 \tag{9}$$

That is, the function $F(x)$ has at least one root somewhere between x_ℓ and x_r. Then split that interval in half

$$x_m = \frac{1}{2}(x_\ell + x_r) \tag{10}$$

If the product $F(x_\ell)F(x_m) < 0$, then a root of $F(x)$ lies between x_ℓ and x_m, otherwise, it lies between x_m and x_r. Repeat until some tolerance ϵ is reached such that

$$|F(x_m)| \leq \epsilon \tag{11}$$

Bisection method

The bisection method is straightforward and reliable, **but it can be slow if you don't have a good initial guess for the interval**.

If there is no root in the chosen interval, then it does not matter what you do.

The method also uses no information whatsoever about the size of the step to take with each iteration. The overall time is determined **only** by the size of the initial interval (i.e. how good your **guess is**) and the tolerance, ϵ.

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We can do better!

Newton's method

The fundamental form of the method alluded to in the last lecture is **Newton's method**. The core of this approach is to use information about the function in order to inform how **big** of a step size to take with each iteration.

Suppose a function $F(x)$ has a root $x = x_0$ and you are within δ of that root at $x = x_0 - \delta$. The question we want to answer is:

How far away from the root are we actually? What is the value of δ?

Using a Taylor expansion (as Wah told us!)

$$F(x_0) = F(x + \delta) \approx F(x) + \delta F'(x) + (O)(\delta^2) \tag{12}$$

By setting $F(x_0)$ by assumption, we can make the linear approximate to $\delta \approx \Delta$ as

$$\Delta = -\frac{F(x)}{F'(x)} \tag{13}$$

Newton's method (II)

Therefore, we can choose a starting point x_i and then update x according to Newton

$$x_{i+1} = x_i + \frac{F(x_i)}{F'(x_i)} \tag{14}$$

The iteration stops after j iterations when

$$|F(x_j)| \leq \epsilon \tag{15}$$